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Optoelectronic properties of the new quaternary chalcogenides Zn2CuInTe4 & Cd2CuInTe4: ab-initio study.

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Abstract: In order to exploit the fundamental properties of the new tellurides quaternary diamond-like structure Zn2CuInTe4 and Cd2CuInTe4, first principles investigation in the frameworkof the Full-Potential LAPW scheme have been carried out for that purpose. We used theWu and Cohen generalized gradient approximation (GGA-WC) to calculate the optimizedstructure that corresponds to the global minima of the energy. Enthalpy of formation showsthat the most stable structures are the relaxed ones. The EV-GGA and the TB-mBJ approx-imations were also used for electronic and optical properties. The equilibrium electronicparameters found are in good agreement with the previous results. The real and thecient, theopt imaginary parts of the dielectric function, the refractive index, the extinction coeffiicalconductivity, the absorption coefficient, the loss function and the reflectivity are reviewedin the large spectral range of photon energy. The present study demonstrates a variety ofnovel electronic and optical properties, which make these compounds highly promising foroptoelectronic materials.

Keywords : DFT, Quaternary tellurides, Enthalpy of formation, band gap, Absorption coefficient